10/521,728B Yong chu 09-05-2007

$%^STN;HighlightOn=;HighlightOff=;

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NEWS 1		Web Page for STN Seminar Schedule - N. America
NEWS 2	MAY 01	New CAS web site launched
NEWS 3	MAY 08	CA/CAplus Indian patent publication number format defined
NEWS 4	MAY 14	RDISCLOSURE on STN Easy enhanced with new search and display fields
NEWS 5	MAY 21	BIOSIS reloaded and enhanced with archival data
NEWS 6	MAY 21	TOXCENTER enhanced with BIOSIS reload
NEWS 7	MAY 21	CA/CAplus enhanced with additional kind codes for German patents
NEWS 8	MAY 22	CA/CAplus enhanced with IPC reclassification in Japanese patents
NEWS 9	JUN 27	CA/CAplus enhanced with pre-1967 CAS Registry Numbers
NEWS 10	JUN 29	STN Viewer now available
NEWS 11	JUN 29	STN Express, Version 8.2, now available
NEWS 12	JUL 02	LEMBASE coverage updated
NEWS 13	JUL 02	LMEDLINE coverage updated
NEWS 14	JUL 02	SCISEARCH enhanced with complete author names
NEWS 15	JUL 02	CHEMCATS accession numbers revised
NEWS 16	JUL 02	CA/CAplus enhanced with utility model patents from China
NEWS 17	JUL 16	CAplus enhanced with French and German abstracts
NEWS 18	JUL 18	CA/CAplus patent coverage enhanced
NEWS 19	JUL 26	USPATFULL/USPAT2 enhanced with IPC reclassification
NEWS 20	JUL 30	USGENE now available on STN
NEWS 21	AUG 06	CAS REGISTRY enhanced with new experimental property tags
NEWS 22	AUG 06	BEILSTEIN updated with new compounds
NEWS 23	AUG 06	FSTA enhanced with new thesaurus edition
NEWS 24	AUG 13	CA/CAplus enhanced with additional kind codes for granted patents
NEWS 25	AUG 20	CA/CAplus enhanced with CAS indexing in pre-1907 records
NEWS 26	AUG 27	Full-text patent databases enhanced with predefined patent family display formats from INPADOCDB
NEWS 27	AUG 27	USPATOLD now available on STN
NEWS 28	AUG 28	CAS REGISTRY enhanced with additional experimental spectral property data

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

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* * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 13:33:33 ON 05 SEP 2007

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

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STRUCTURE FILE UPDATES:     4 SEP 2007  HIGHEST RN 946048-22-2
DICTIONARY FILE UPDATES:    4 SEP 2007  HIGHEST RN 946048-22-2

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

  Please note that search-term pricing does apply when
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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document.  For information
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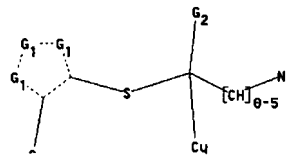

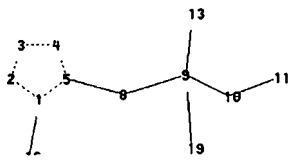

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ring nodes :
1 2 3 4 5
chain bonds :
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ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-16 2-3 3-4 4-5 5-8 8-9 9-10 9-13 9-19 10-11

G1:C,S

G2:H,CH3,Et,n-Pr,n-Bu

G3:X,MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 8:CLASS 9:CLASS 10:CLASS 11:CLASS
13:CLASS
16:CLASS 19:Atom
Generic attributes :
19:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 13:34:26 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5668 TO ITERATE

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 35.3% PROCESSED     2000 ITERATIONS                                  0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       108846 TO   117874
PROJECTED ANSWERS:               0 TO        0

L2             0 SEA SSS SAM L1

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FULL SEARCH INITIATED 13:34:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   112533 TO ITERATE

100.0% PROCESSED   112533 ITERATIONS                                  7 ANSWERS
SEARCH TIME: 00.00.06

L3             7 SEA SSS FUL L1

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COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   172.55     172.76

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FILE COVERS 1907 - 5 Sep 2007  VOL 147 ISS 11
FILE LAST UPDATED: 4 Sep 2007  (20070904/ED)

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=> s l3
L4             2 L3                                   Not ODP.

=> d ibib abs hitstr tot

L4   ANSWER 1 OF 2  CAPLUS  COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER:         2004:80678  CAPLUS  Full-text
DOCUMENT NUMBER:          140:145993
TITLE:                    Preparation of aminohydroxyalkylthiothiophenecarbonitr
                          iles as nitric oxide synthase (NOS) inhibitors.
```

INVENTOR(S): Mete, Antonio; Walters, Iain
PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
SOURCE: PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004009580	A1	20040129	WO 2003-SE1215	20030715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003245230	A1	20040209	AU 2003-245230	20030715
EP 1539731	A1	20050615	EP 2003-738863	20030715
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JP 2006504655	T	20060209	JP 2004-522890	20030715
US 2005203172	A1	20050915	US 2005-521727	20050118
PRIORITY APPLN. INFO.:			SE 2002-2279 A	20020719
			WO 2003-SE1215 W	20030715

OTHER SOURCE(S): MARPAT 140:145993
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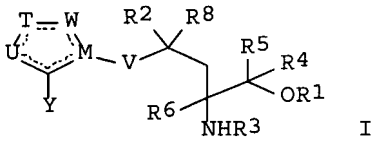


I

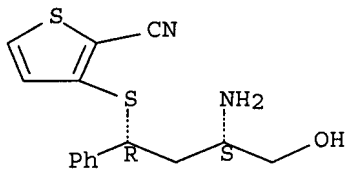
AB Title compds. [I; Y = (fluoro)alkyl, (fluoro)alkoxy, halo, CN, C:CH, NO2, CH2OH, CHO, Ac, NH2, NHCHO, NHCOCH3, NHSO2Me; T, U, W = CX, N, NR13, O, SOm; m = 0-2; X = H, (fluoro)alkyl, (fluoro)alkoxy, halo, OH, SH, CN, C:CH, N(R14)2, NO2, CH2OH, CHO, Ac, NHCHO; V = NR7, O, CH2, SOn, CH2O, CH2NR7, CH2SOn, CH2CH2, CH:CH; n = 0-2; M = C, N; R1, R8 = H, Me.; R2 = alkyl, alkenyl, alkynyl, cycloalkyl, 4-8 membered satd. heterocyclyl incorporating 1 O, S, N; any of said groups being optionally further substituted by alkyl, alkoxy, alkylthio, cycloalkyl, halo, (substituted) Ph; or R2 = (substituted) Ph, 5-6 membered heteroaryl contg. 1-3 O, S, N; R3 = H, (substituted) alkyl, cycloalkyl; R4-R7, R9-R12, R14 = H, alkyl; R13 = H, alkyl, CHO, Ac, SO2CH3, CF3], were prepd. Thus, 1,1-dimethylethyl (4S)-4-((2R)-2-mercapto-2-phenylethyl)-2,2-dimethyl-3- oxazolidinecarboxylate (prepn. given), 3-bromothiophene-2-carbonitrile, and NaH were stirred 24 h in DMF to give 1,1-dimethylethyl (4S)-4-[(2R)-2-[(2-cyano-3-thienyl)thio]-2-phenylethyl]-2,2-dimethyl-3- oxazolidinecarboxylate. The latter was stirred 2 h with 4M HCl in dioxane to give a residue which was treated with oxalic acid in Et2O to give

3-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-2-thiophenecarbonitrile oxalate. I inhibited iNOS with IC50 <10 .mu.M.

IT 651353-83-2P 651353-84-3P 651353-85-4P
651353-86-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminohydroxyalkylthiothiophenecarbonitriles as nitric oxide synthase inhibitors)

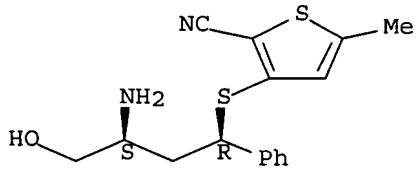
RN 651353-83-2 CAPLUS
CN 2-Thiophenecarbonitrile, 3-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 651353-84-3 CAPLUS
CN 2-Thiophenecarbonitrile, 3-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-5-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 651353-85-4 CAPLUS
CN 2-Thiophenecarbonitrile, 3-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

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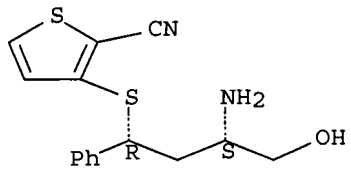
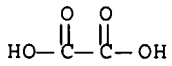
CRN 651353-83-2
CMF C15 H16 N2 O S2

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

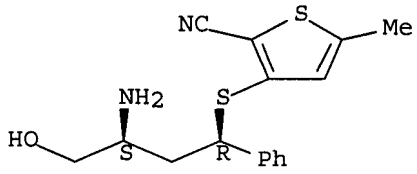


RN 651353-86-5 CAPLUS
CN 2-Thiophenecarbonitrile, 3-[[(1R,3S)-3-amino-4-hydroxy-1-phenylbutyl]thio]-5-methyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 651353-84-3
CMF C16 H18 N2 O S2

Absolute stereochemistry.



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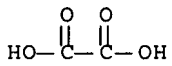
CRN 144-62-7
CMF C2 H2 O4



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:80677 CAPLUS Full-text
DOCUMENT NUMBER: 140:128265
TITLE: Preparation of 3-[((1S)-2-amino-1-phenylethyl)thio]-5-methyl-2-thiophenecarbonitrile oxalate and related compounds as nitric oxide synthase inhibitors.

INVENTOR(S): Mete, Antonio; Walters, Iain
PATENT ASSIGNEE(S): Astrazeneca Ab, Swed.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004009579	A1	20040129	WO 2003-SE1214		20030715
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
AU 2003251259	A1	20040209	AU 2003-251259		20030715
EP 1539732	A1	20050615	EP 2003-765417		20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
JP 2005537281	T	20051208	JP 2004-522889		20030715
US 2006019999	A1	20060126	US 2005-521728		20050118
PRIORITY APPLN. INFO.:			SE 2002-2280	A	20020719
			WO 2003-SE1214	W	20030715

OTHER SOURCE(S): MARPAT 140:128265
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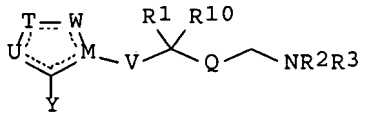

I

AB Title compds. [I; Y = (F-substituted) alkyl, alkoxy, halo, CN, C:CH, NO2, CH2OH, CHO, Ac, NH2, NHCHO, NHAc, NHSO2Me; T, U, W = CX, N, NR9, O, S(O)m, .gtoreq.1 of T, U, W must = heteroatom and .ltoreq.1 of T, U and W may = NR9, O, SOm; m, n = 0-2; X = H, (F-substituted) alkyl, alkoxy, halo, OH, SH, CN, C:CH, N(R11)2, NO2, CH2OH, CHO, Ac, NHCHO; V = NR4, O, CH2, SOn, OCH2, CH2O, NR4CH2, CH2NR4, CH2SOn, SOnCH2, CH2CH2, CH:CH; M = C, and when M is bonded to a CH2 moiety in V, then M may = N; R10 = H, Me. Q = (CH2)p; p = 0-3; R1 = (substituted) Ph, 5-6 membered heteroaryl contg. 1-3 O, S and N; R2, R3 = H, (substituted) alkyl, cycloalkyl; Z = CO, bond; R4, R11 = H, alkyl; R5-R8 = H, alkyl; R9 = H, alkyl, CHO, Ac, SO2Me, CF3], were prepd. Thus, S-[(1S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-1- phenylethyl]benzenecarbothioate (prepn. given) was stirred 2h with aq. NH3 in MeOH; the residue was stirred with 3-bromo-5-methyl-2- thiophenecarbonitrile (prepn. given) and Cs2CO3 in DMF for 24 h to give 1,1-dimethylethyl [(2S)-2-[(2-cyano-5-methyl-3-thienyl)thio]-2- phenylethyl]carbamate. The latter was stirred with 4M HCl in dioxane at 20.degree. for 2 h and the residue was treated with oxalic acid in Et2O to give 3-[((1S)-2-amino-1-phenylethyl)thio]-5-methyl-2-

thiophenecarbonitrile oxalate. The latter inhibited nitric oxide synthase with IC50 <100 .mu.M.

IT 651034-24-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of aminophenylethylthiomethylthiophenecarbonitrile and related compds. as nitric oxide synthase inhibitors)

RN 651034-24-1 CAPLUS

CN 2-Thiophenecarbonitrile, 3-[[(1S)-2-amino-1-phenylethyl]thio]-5-methyl-, ethanedioate (9CI) (CA INDEX NAME)

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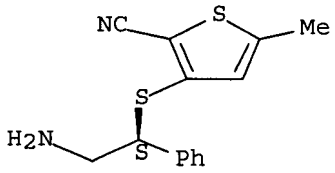
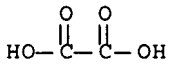
CRN 651034-23-0
CMF C14 H14 N2 S2

Absolute stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4

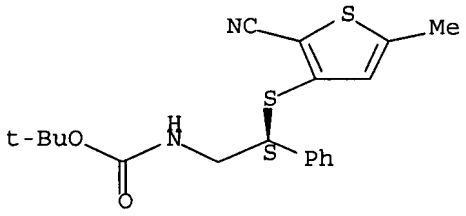


IT 651034-45-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of aminophenylethylthiomethylthiophenecarbonitrile and related compds. as nitric oxide synthase inhibitors)

RN 651034-45-6 CAPLUS

CN Carbamic acid, [(2S)-2-[(2-cyano-5-methyl-3-thienyl)thio]-2-phenylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	21.82	194.58

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-1.56	-1.56

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STRUCTURE FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2
DICTIONARY FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

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TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

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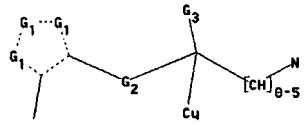
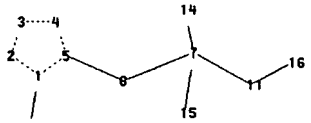
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R.str





chain nodes :
6 7 8 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
1-8 5-6 6-7 7-11 7-14 7-15 11-16
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,S,N,CH2

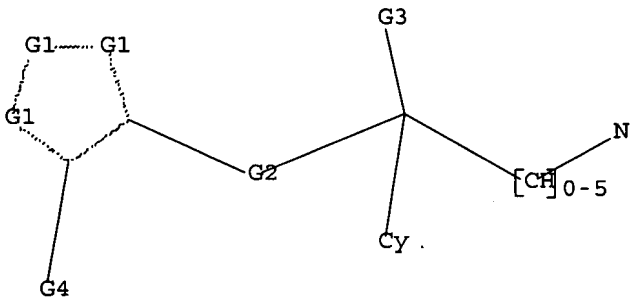
G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom
14:CLASS
15:Atom 16:CLASS
Generic attributes :
15:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L5 STRUCTURE UPLOADED

=> d
L5 HAS NO ANSWERS
L5 STR



G1 C,S
G2 O,S,N,CH2
G3 H,Me,Et,n-Pr,n-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l5
SAMPLE SEARCH INITIATED 13:49:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   735141 TO ITERATE

  0.3% PROCESSED     2000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     14655654 TO 14749986
PROJECTED ANSWERS:               0 TO        0

L6             0 SEA SSS SAM L5

=> s l5 full
FULL SEARCH INITIATED 13:50:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 14703568 TO ITERATE

  1.9% PROCESSED   272888 ITERATIONS                                 0 ANSWERS

  3.7% PROCESSED   548769 ITERATIONS                                 0 ANSWERS

  5.1% PROCESSED   745208 ITERATIONS                                 0 ANSWERS

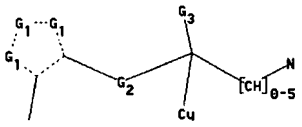
  6.6% PROCESSED   973220 ITERATIONS                                 0 ANSWERS

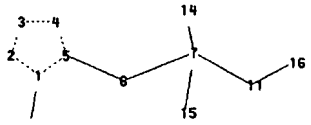
  6.8% PROCESSED  1000000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.01.12

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     14703568 TO 14703568
PROJECTED ANSWERS:               0 TO        0

L7             0 SEA SSS FUL L5
```

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728R-1.str





chain nodes :
6 7 8 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
1-8 5-6 6-7 7-11 7-14 7-15 11-16
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,N,CH2

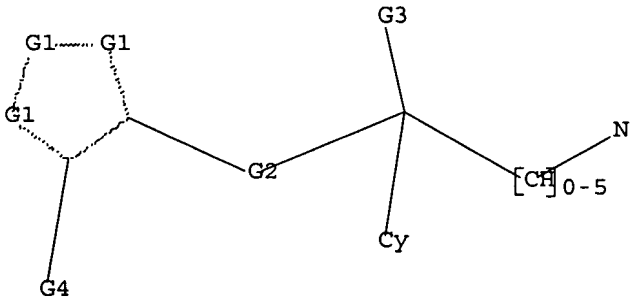
G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom
14:CLASS
15:Atom 16:CLASS
Generic attributes :
15:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L8 STRUCTURE UPLOADED

=> d
L8 HAS NO ANSWERS
L8 STR



G1 C,S
G2 O,N,CH2
G3 H,Me,Et,n-Pr,n-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l8
SAMPLE SEARCH INITIATED 13:53:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 722979 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.04

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 14412733 TO 14506427
PROJECTED ANSWERS: 0 TO 0

L9 0 SEA SSS SAM L8

=>
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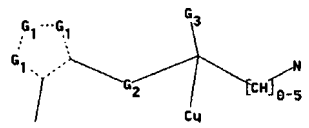
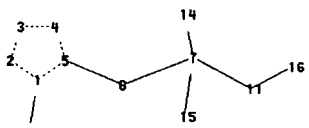




chain nodes :
6 7 8 11 14 15 16
ring nodes :
1 2 3 4 5
chain bonds :
1-8 5-6 6-7 7-11 7-14 7-15 11-16

ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-8 2-3 3-4 4-5 5-6 6-7 7-11 7-14 7-15 11-16

G1:C,S

G2:O,N

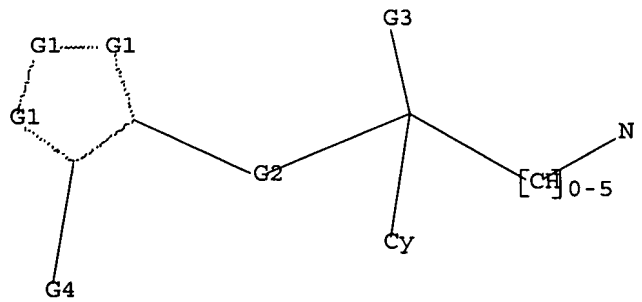
G3:H,CH3,Et,n-Pr,n-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:Atom
14:CLASS
15:Atom 16:CLASS
Generic attributes :
15:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L10 STRUCTURE UPLOADED

=> d
L10 HAS NO ANSWERS
L10 STR



G1 C,S
G2 O,N
G3 H,Me,Et,n-Pr,n-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l10
SAMPLE SEARCH INITIATED 13:54:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 572155 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS 0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 11400624 TO 11485576
PROJECTED ANSWERS: 0 TO 0

L11 0 SEA SSS SAM L10

=>
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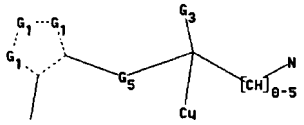
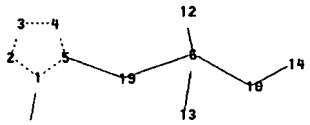




chain nodes :
6 7 10 12 13 14 19
ring nodes :
1 2 3 4 5
chain bonds :
1-7 5-19 6-13 6-10 6-12 6-19 10-14
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-7 2-3 3-4 4-5 5-19 6-13 6-10 6-12 6-19 10-14

G1:C,S

G3:H,CH3,Et,n-Pr,n-Bu

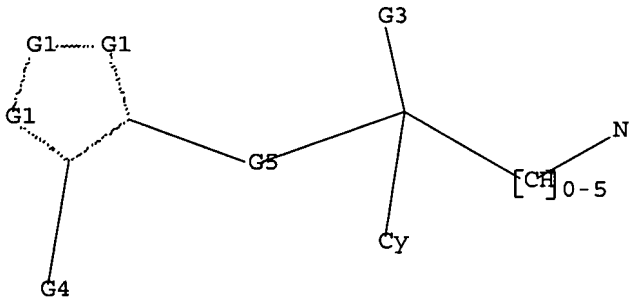
G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

G5:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 10:Atom 12:CLASS
13:Atom
14:CLASS 19:CLASS
Generic attributes :
13:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L12 STRUCTURE UPLOADED

=> d
L12 HAS NO ANSWERS
L12 STR



G1 C,S
G2
G3 H,Me,Et,n-Pr,n-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2
G5 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l12
SAMPLE SEARCH INITIATED 13:56:42 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 572155 TO ITERATE

0.3% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: 11400624 TO 11485576
PROJECTED ANSWERS: 0 TO 0

L13 0 SEA SSS SAM L12

=>
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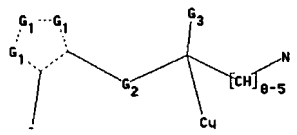
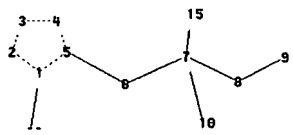




chain nodes :
6 7 8 9 10 15 20
ring nodes :
1 2 3 4 5
chain bonds :
1-20 5-6 6-7 7-8 7-10 7-15 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-20 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-15 8-9

G1:C,S

G2:O,N,CH2

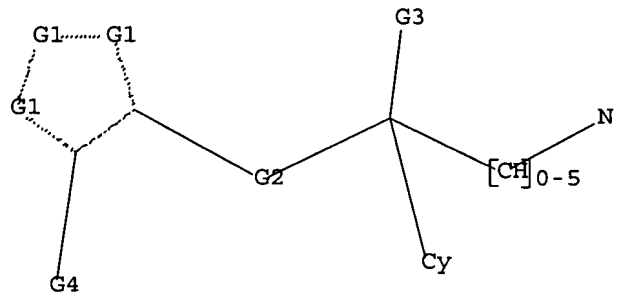
G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
15:CLASS 20:CLASS
Generic attributes :
10:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L14 STRUCTURE UPLOADED

=> d
L14 HAS NO ANSWERS
L14 STR



G1 C,S
G2 O,N,CH2
G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l14
SAMPLE SEARCH INITIATED 14:00:56 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   722979 TO ITERATE

  0.3% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.03

FULL FILE PROJECTIONS:  ONLINE  **INCOMPLETE**
                        BATCH   **INCOMPLETE**
PROJECTED ITERATIONS:     14412733 TO 14506427
PROJECTED ANSWERS:               0 TO        0

L15           0 SEA SSS SAM L14

=>
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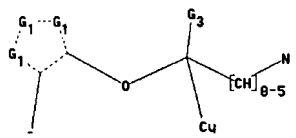
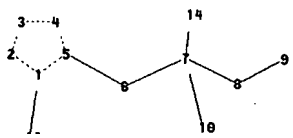
```






```
chain nodes :
6  7  8  9  10  14  19
ring nodes :
1  2  3  4  5
chain bonds :
1-19  5-6  6-7  7-8  7-10  7-14  8-9
ring bonds :
1-2  1-5  2-3  3-4  4-5
exact/norm bonds :
1-2  1-5  1-19  2-3  3-4  4-5  5-6  6-7  7-8  7-10  7-14  8-9


G1:C,S

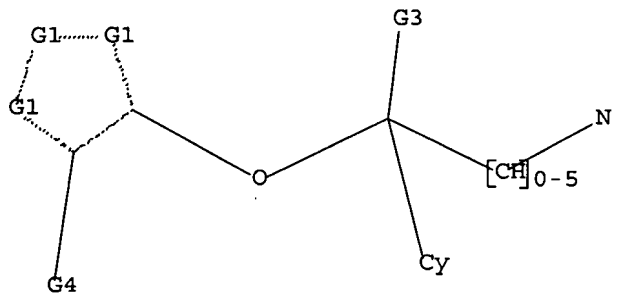
G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:CLASS  7:CLASS  8:CLASS  9:CLASS  10:Atom
14:CLASS  19:CLASS
Generic attributes :
10:
Saturation              : Unsaturated
Number of Carbon Atoms : less than 7
```

L16 STRUCTURE UPLOADED

=> d
L16 HAS NO ANSWERS
L16 STR



G1 C,S
G2
G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l16
SAMPLE SEARCH INITIATED 14:02:23 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 30976 TO ITERATE

6.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 608996 TO 630044
PROJECTED ANSWERS: 0 TO 0

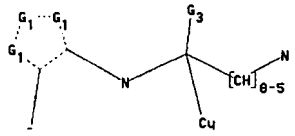
L17 0 SEA SSS SAM L16

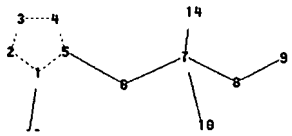
=> s l16 full
FULL SEARCH INITIATED 14:02:32 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 614816 TO ITERATE

100.0% PROCESSED 614816 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.06

L18 0 SEA SSS FUL L16

=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-2.str





chain nodes :
6 7 8 9 10 14 19
ring nodes :
1 2 3 4 5
chain bonds :
1-19 5-6 6-7 7-8 7-10 7-14 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

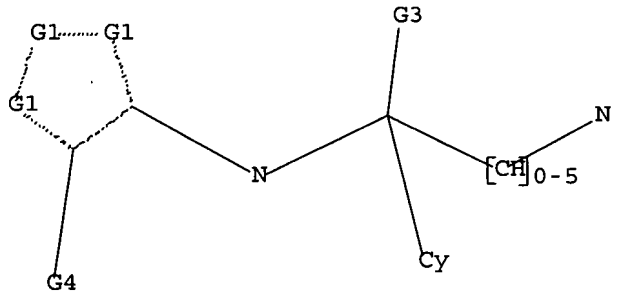
G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom
14:CLASS 19:CLASS
Generic attributes :
10:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L19 STRUCTURE UPLOADED

=> d
L19 HAS NO ANSWERS
L19 STR



G1 C,S
G2
G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

```
=> s l19
SAMPLE SEARCH INITIATED 14:03:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -    45149 TO ITERATE

  4.4% PROCESSED     2000 ITERATIONS                                0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       890294 TO   915666
PROJECTED ANSWERS:               0 TO        0

L20            0 SEA SSS SAM L19

=> s l19 full
FULL SEARCH INITIATED 14:03:40 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   909705 TO ITERATE

100.0% PROCESSED   909705 ITERATIONS                               2 ANSWERS
SEARCH TIME: 00.00.15

L21            2 SEA SSS FUL L19

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                              525.75     720.33

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)    SINCE FILE      TOTAL
                                                   ENTRY    SESSION
CA SUBSCRIBER PRICE                                0.00      -1.56

FILE 'CAPLUS' ENTERED AT 14:04:07 ON 05 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
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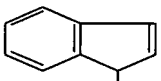
FILE COVERS 1907 - 5 Sep 2007 VOL 147 ISS 11
FILE LAST UPDATED: 4 Sep 2007 (20070904/ED)

=> s l21
L22 1 L21

=> d ibib abs hitstr tot

L22 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1984:191517 CAPLUS Full-text
DOCUMENT NUMBER: 100:191517
TITLE: Reactions of some arylmethylenedicarbamates with ethyl vinyl ether
AUTHOR(S): Sirotanovic-Maletic, Ksenija; Bajlon-Pastor, Milka; Markovic, Rade
CORPORATE SOURCE: Fac. Sci., Univ. Belgrade, Belgrade, YU-11001, Yugoslavia
SOURCE: Glasnik Hemijskog Drustva Beograd (1983), 48(7), 401-8
CODEN: GHDBAX; ISSN: 0017-0941
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 100:191517
GI

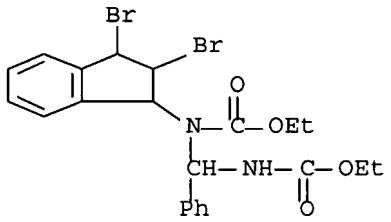


N(CO2Et)CHPhNHCO2Et IV

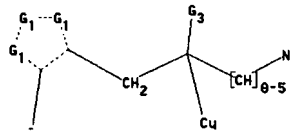
AB The title dicarbamates, RC6H4CH(NHCO2R1)2 (I; R1 = Et, R = H, 2-, 3-Cl, 2-, 4-MeO; R1 = Me2CHCH2, R = H, 2-, 3-, 4- Cl), condense with EtOCH:CH2 (II) in the presence of 1-2% BF3.Et2O (III) to give tricarbamates RC6H4CH(NHCO2R1) CH2CH(NHCO2R1)2. Electron-withdrawing substituents impede the reaction; I (R = NO2) do not react under these conditions. With an excess of III present, I (R = H, R1 = Et) reacted with II to give indan IV.

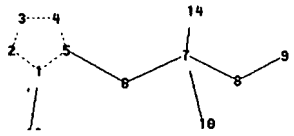
IT 89950-54-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 89950-54-9 CAPLUS

CN Carbamic acid, (2,3-dibromo-2,3-dihydro-1H-inden-1-yl)[[(ethoxycarbonyl)amino]phenylmethyl]-, ethyl ester (9CI) (CA INDEX NAME)



=>
Uploading C:\Documents and Settings\ychu\Desktop\Case\10521728\10521728S-3str.str





chain nodes :
6 7 8 9 10 14 19
ring nodes :
1 2 3 4 5
chain bonds :
1-19 5-6 6-7 7-8 7-10 7-14 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

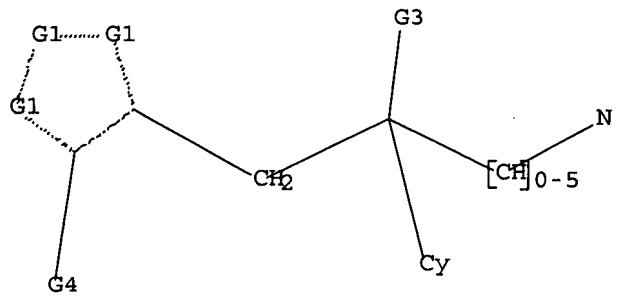
G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 14:CLASS 19:CLASS
Generic attributes :
10:
Saturation : Unsaturated

Number of Carbon Atoms : less than 7

L23 STRUCTURE UPLOADED

=> d
L23 HAS NO ANSWERS
L23 STR



G1 C,S
G2
G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l23
REGlstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

SAMPLE SEARCH INITIATED 14:05:54 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 44548 TO ITERATE

4.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 878358 TO 903562
PROJECTED ANSWERS: 0 TO 0

L24 0 SEA SSS SAM L23

L25 0 L24

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.47	727.93

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'CAPLUS' ENTERED AT 14:06:02 ON 05 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 5 Sep 2007 VOL 147 ISS 11
FILE LAST UPDATED: 4 Sep 2007 (20070904/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.47	728.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

FILE 'REGISTRY' ENTERED AT 14:06:08 ON 05 SEP 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2
DICTIONARY FILE UPDATES: 4 SEP 2007 HIGHEST RN 946048-22-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>
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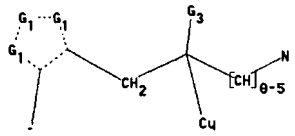
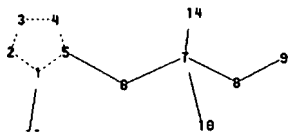




chain nodes :
6 7 8 9 10 14 19
ring nodes :
1 2 3 4 5
chain bonds :
1-19 5-6 6-7 7-8 7-10 7-14 8-9
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 1-19 2-3 3-4 4-5 5-6 6-7 7-8 7-10 7-14 8-9

G1:C,S

G3:H,CH3,Et,n-Pr,i-Pr,n-Bu,s-Bu

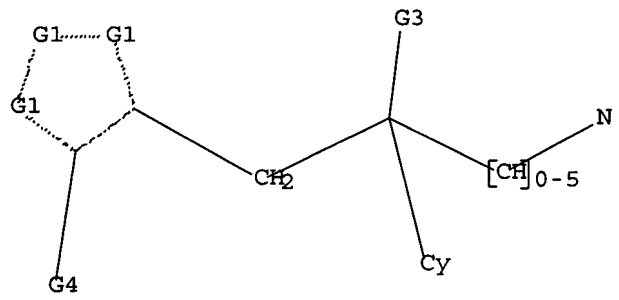
G4:X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:Atom 14:CLASS 19:CLASS
Generic attributes :
10:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7

L26 STRUCTURE UPLOADED

=> d
L26 HAS NO ANSWERS

L26 STR



G1 C,S
G2
G3 H,Me,Et,n-Pr,i-Pr,n-Bu,s-Bu
G4 X,MeO,EtO,n-PrO,i-PrO,n-BuO,s-BuO,CN,CHO,NH,NH2,NO2

Structure attributes must be viewed using STN Express query preparation.

=> s l26
SAMPLE SEARCH INITIATED 14:06:39 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 44548 TO ITERATE

4.5% PROCESSED 2000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 878358 TO 903562
PROJECTED ANSWERS: 0 TO 0

L27 0 SEA SSS SAM L26

=> s l26 full
FULL SEARCH INITIATED 14:06:46 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 894122 TO ITERATE

100.0% PROCESSED 894122 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.10

L28 0 SEA SSS FUL L26

=>

=>
Executing the logoff script...

=> LOG H

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.00	901.40

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.34

SESSION WILL BE HELD FOR 120 MINUTES
STN INTERNATIONAL SESSION SUSPENDED AT 14:07:47 ON 05 SEP 2007